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Title :
First Principles Studies on Properties of Pb(II), Sn(II) and Ge(II) Ferroelectric Materials Using Density Functional Theory

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Quantum calculations via the first-principles study using the density functional theory (DFT) have offered great opportunities to describe the origin and most fundamental properties of new materials. In addition, detailed properties of the materials can be visualized by providing an accurate view at the atomic level. In this study, works are focused on investigating new lead-free ferroelectric materials that have a similar special ns^2 lone pair electrons with Pb (II) such as Sn (II) and Ge (II) via first principles calculation. Modification of Pb-based materials (PTO and PZT) by substituting or doping at the A-site are numerically anticipated to enhance the ferroelectric properties as well as to eventually reduce the consumption of Pb (II) in electroactive devices. Properties of lead-based materials $PbTiO_3$ (PTO), $PbZrO_3$ (PZO) and $PbZrTiO_3$ (PZT) as reference materials were compared with new lead-free ferroelectric materials such as $SnTiO_3$ (SnTO), $GeTiO_3$ (GTO) and $SnZrO_3$ (SnZO). All calculations were performed using first principles study based on Density Functional Theory (DFT) that has been implemented in CASTEP computer code. Functional GGA-PBEsol exhibits the most accurate values for lattice parameter with 0.6 % relative to experimental values for both cubic $PbTiO_3$ and $PbZrO_3$ (reference materials). Meanwhile, LDA-CAPZ functional is accurate for tetragonal PTO. The elastic properties values confirm that cubic PTO, SnTO, GTO, SnZO and PZO as well as tetroganal PTO, SnTO and GTO are mechanically stable. The electronic band structure, density of states (DOS) and electron density variation indicate the existence of hybridizations between anion O 2p and cation Pb 6s/ Sn 5s/Ge 4s (special lone pair) in tetragonal PTO, SnTO, GTO and SnZO phase. Optical results show that anion O 2p, cation Pb 6p, Sn 5p , Ge 4p and Ti 3d, Zr 4d states respectively correspond to the transition electrons from valence states to the bottom of conduction state of the $ATiO_3$ (A=Pb, Sn, Ge) and $AZrO_3$ (A=Pb, Sn). The phonon calculation and cohesive energy revealed that the PTO and SnTO are stable in the tetragonal P4mm phase compared to the non polar ilmenite structure. However, $GeTiO_3$ apparently shows non-polar ilmenite structure is more stable compared to the ferroelectric perovskite structure. The phonon dispersion analyses for PZO and SnZO proves that both compounds have ground state structure with antiferroelectric orthorhombic (Pbam, no: 55 space group) and in approximation with the polar ferroelectric phase rhombohedral (R3c, no: 161 space group). In this work, calculations on novel compounds consist of Sn (II) and Ge (II) in PTO and Sn (II) in PZT provide new insights on geometrical and electronic structure of materials. Thus, these findings will be able to gear up efforts in reducing lead consumption by substituting or doping Sn and Ge in Pb-based system, and hence will substantially contribute to greener environment.